Gradient Descent

Nipun Batra

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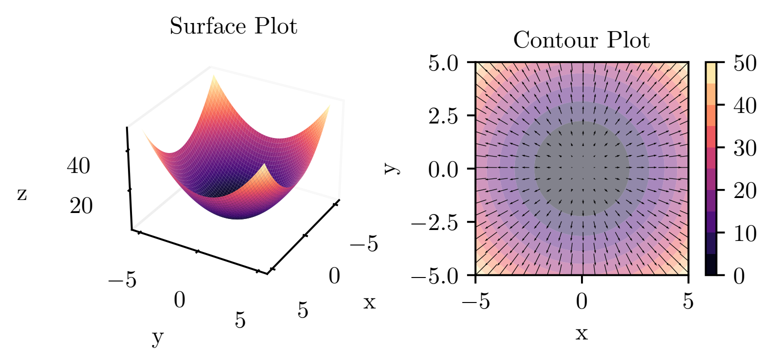
IIT Gandhinagar

Revision

Contour Plot And Gradients

$z = f(x, y) = x^2 + y^2$



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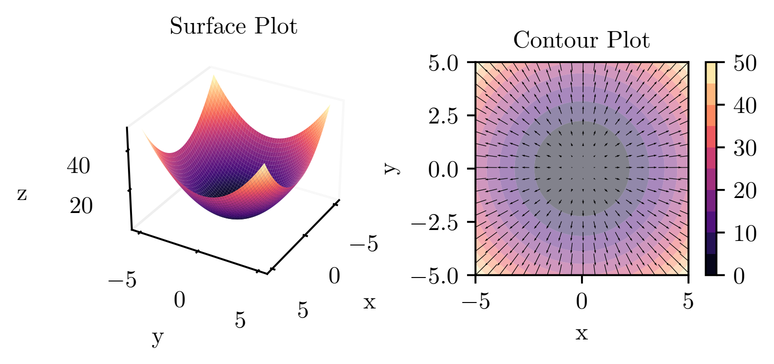

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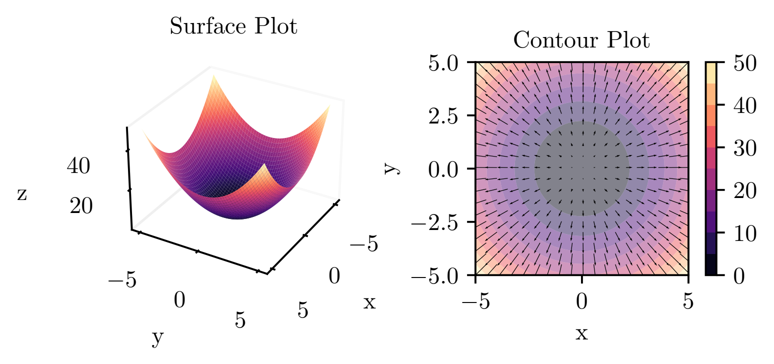

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$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

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Optimization algorithms

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- Goal:

$$\theta^* = \arg\min_{\theta} f(\theta) \tag{2}$$

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- It is a local search algorithm/greedy

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    - $\theta_i \leftarrow \theta_{i-1} - \alpha \nabla f(\theta_{i-1})$

Taylor's Series

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- The vector form of the above equation is given by:

$$f(\vec{x}) = f(\vec{x_0}) + \nabla f(\vec{x_0})^T(\vec{x} - \vec{x_0}) + \frac{1}{2}(\vec{x} - \vec{x_0})^T \nabla^2 f(\vec{x_0})(\vec{x} - \vec{x_0}) + \dots \quad (4)$$

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- where $\nabla^2 f(\vec{x_0})$ is the Hessian matrix and $\nabla f(\vec{x_0})$ is the gradient vector

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- $f(x) = 1 + 0(x-0) + \frac{-1}{2!}(x-0)^2 = 1 - \frac{x^2}{2}$

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- First order Taylor's series approximation is given by:
- $f(x) = f(x_0) + f'(x_0)(x - x_0) = 6 + 4(x - 2) = 4x - 2$

Taylor's Series (Alternative form)

- We have:

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \ldots \quad (5)$$

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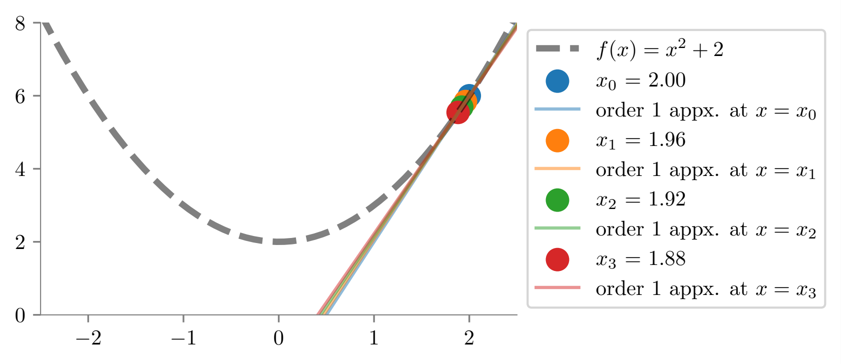
- This is the gradient descent algorithm: $\vec{x_1} = \vec{x_0} - \alpha\nabla f(\vec{x_0})$

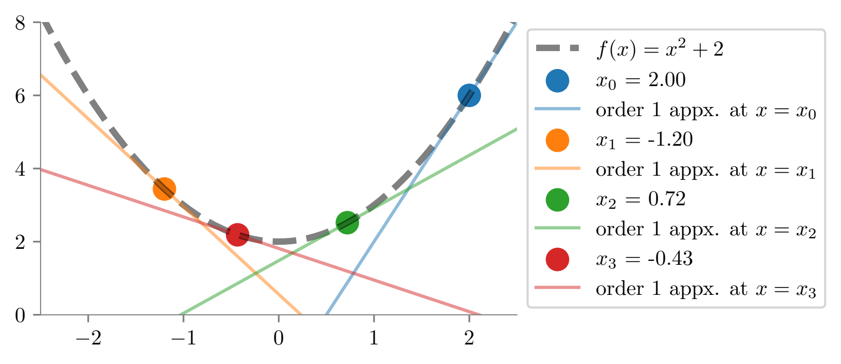
Effect of learning rate

Low learning rate $\alpha = 0.01$: Converges slowly



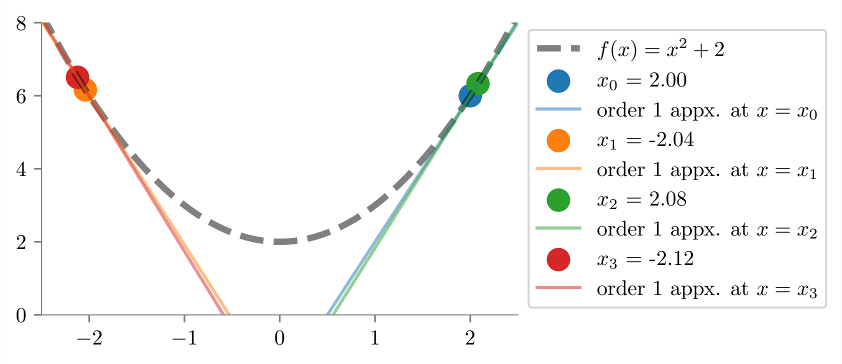
Effect of learning rate

High learning rate $\alpha = 0.8$: Converges quickly, but might overshoot



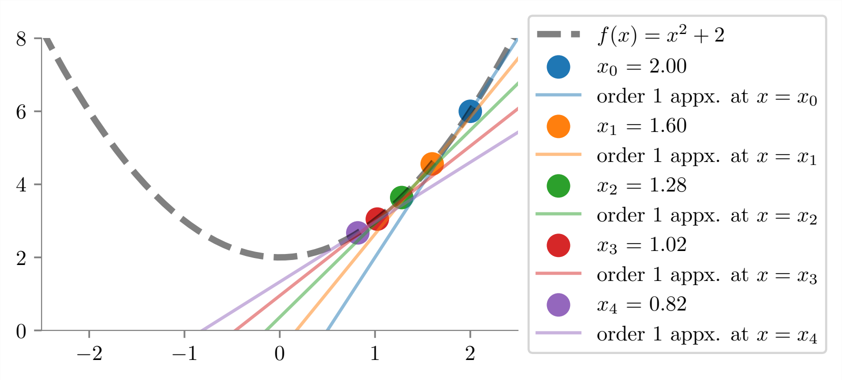
Effect of learning rate

Very high learning rate $\alpha = 1.01$: Diverges



Effect of learning rate

Appropriate learning rate $\alpha = 0.1$



Gradient Descent for linear regression

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- Mean Squared Error $MSE(\theta) = \frac{1}{N}\sum_{i=1}^{N}\left(f\left(x_i|\theta\right) - y_i\right)^2$
- **Objective function** is the most general term for any function that you optimize during training.

Gradient Descent : Example

Learn $y = \theta_0 + \theta_1 x$ on following dataset, using gradient descent where initially $(\theta_0, \theta_1) = (4, 0)$ and step-size, $\alpha = 0.1$, for 2 iterations.

x	**y**
1	1
2	2
3	3

Gradient Descent : Example

Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

Error for i^{th} datapoint, $\epsilon_i = y_i - \hat{y}_i$

$\epsilon_1 = 1 - \theta_0 - \theta_1$

$\epsilon_2 = 2 - \theta_0 - 2\theta_1$

$\epsilon_3 = 3 - \theta_0 - 3\theta_1$

$$\text{MSE} = \frac{\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2}{3} = \frac{14 + 3\theta_0^2 + 14\theta_1^2 - 12\theta_0 - 28\theta_1 + 12\theta_0\theta_1}{3}$$

Difference between SSE and MSE

$$\sum \epsilon_i^2 \textit{ increases as the number of examples increase}$$

So, we use MSE

$$MSE = \frac{1}{n} \sum \epsilon_i^2$$

Here n denotes the number of samples

Gradient Descent : Example

$$\frac{\partial MSE}{\partial \theta_0} = \frac{2\sum_i (y_i - \theta_0 - \theta_1 x_i)(-1)}{N} = \frac{2\sum_i \epsilon_i (-1)}{N}$$

$$\frac{\partial MSE}{\partial \theta_1} = \frac{2\sum_i (y_i - \theta_0 - \theta_1 x_i)(-x_i)}{N} = \frac{2\sum_i \epsilon_i (-x_i)}{N}$$

Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.2 \frac{((1-(4+0))(-1) + (2-(4+0))(-1) + (3-(4+0))(-1))}{3}$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

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$$\theta_1 = 0 - 0.2\frac{((1-(4+0))(-1)+(2-(4+0))(-2)+(3-(4+0))(-3))}{3}$$

$$\theta_1 = -0.67$$

Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.2 \frac{((1-(3.6-0.67))(-1)+(2-(3.6-0.67\times 2))(-1)+(3-(3.6-0.67\times 3))(-1))}{3}$$

$$\theta_0 = 3.54$$

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Gradient Descent : Example

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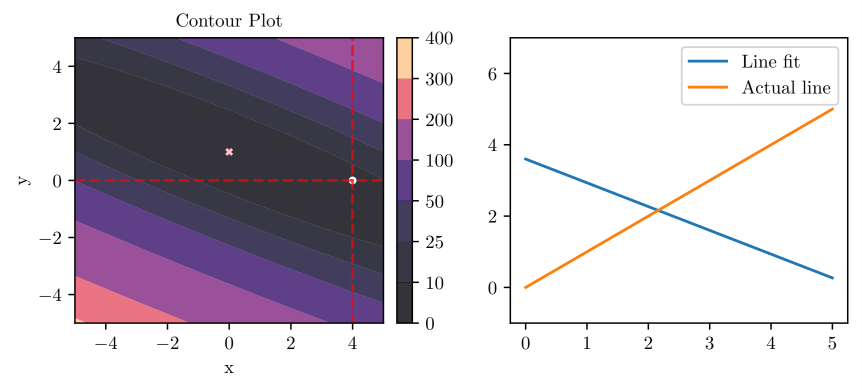
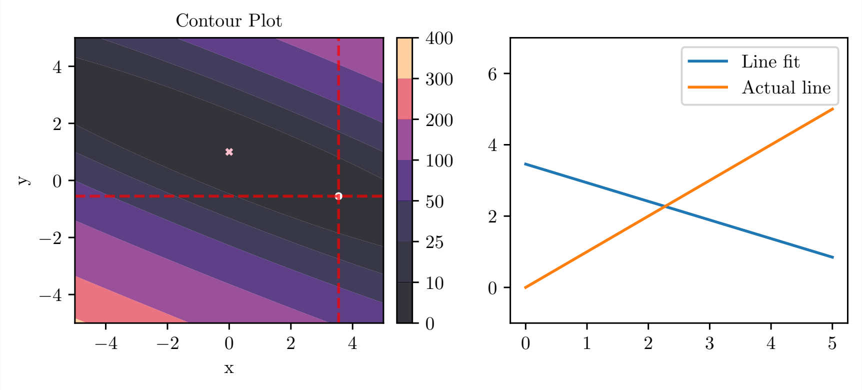
$$\theta_0 = -0.55$$

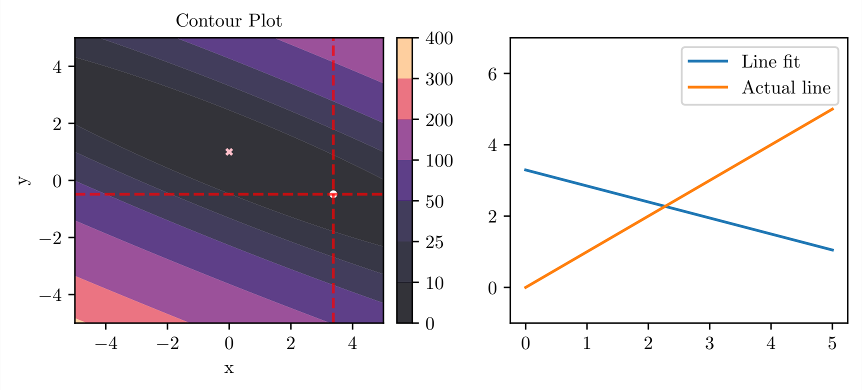
Gradient Descent : Example (Iteraion 0)



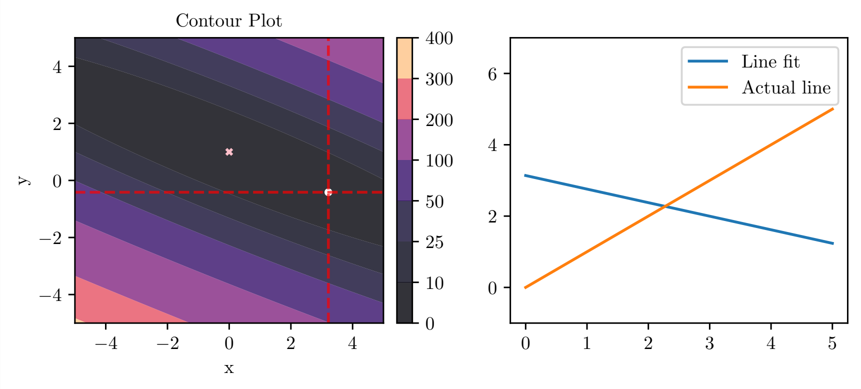
Gradient Descent : Example (Iteraion 2)



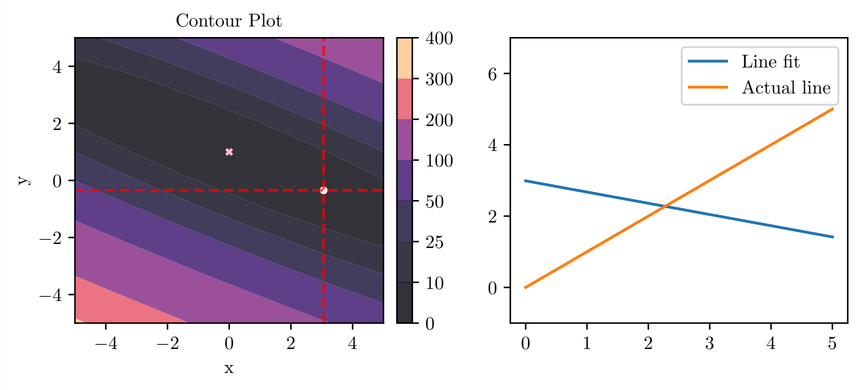
Gradient Descent : Example (Iteraion 4)



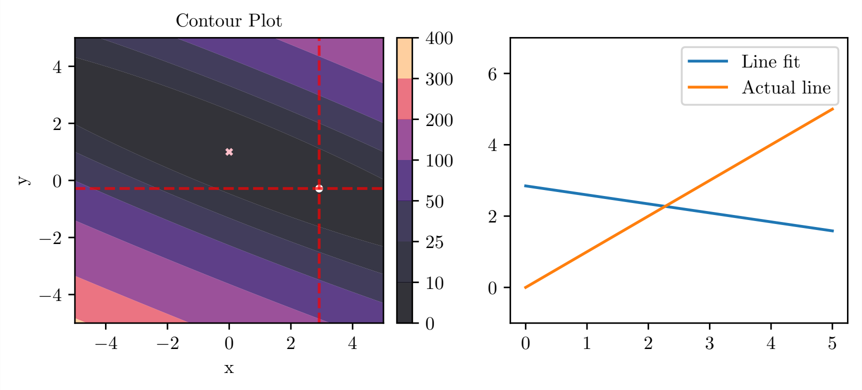
Gradient Descent : Example (Iteraion 6)



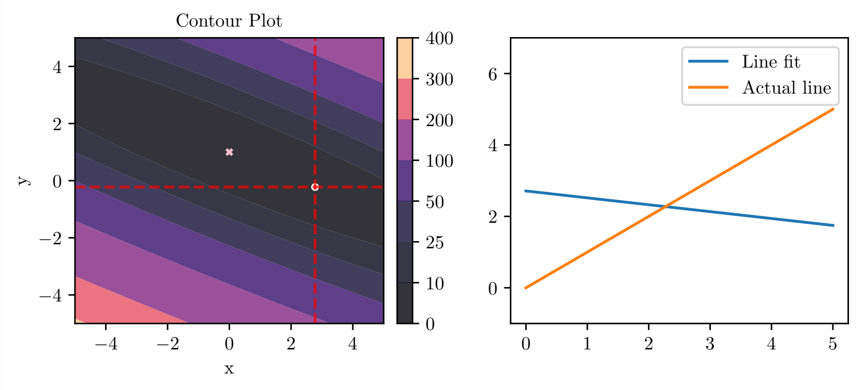
Gradient Descent : Example (Iteraion 8)



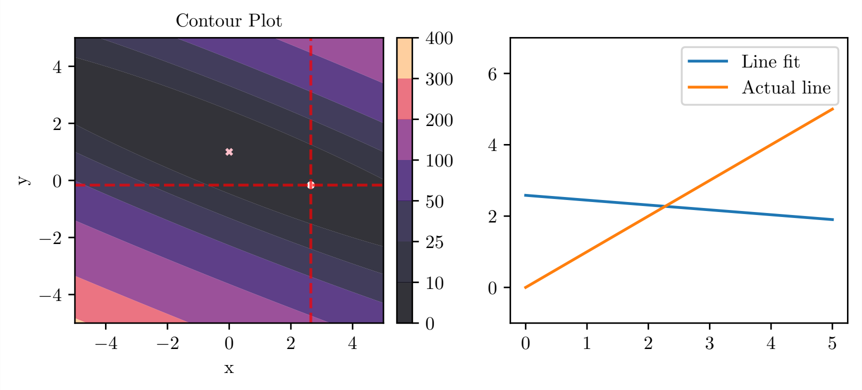
Gradient Descent : Example (Iteraion 10)



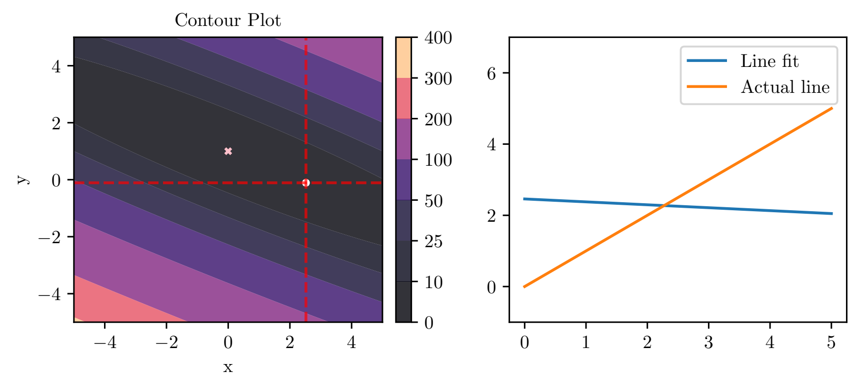
Gradient Descent : Example (Iteraion 12)



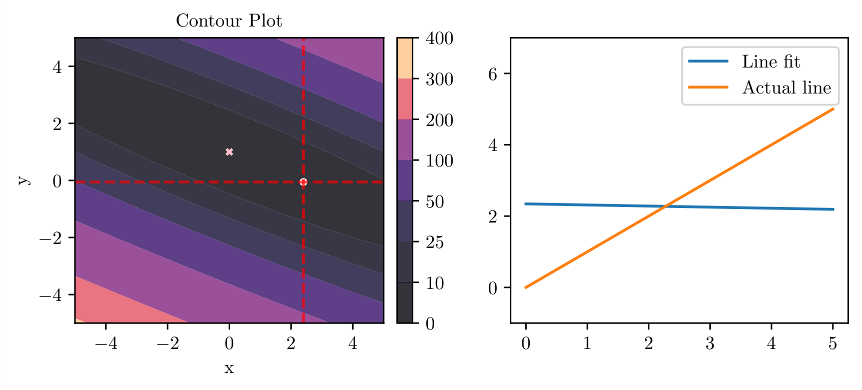
Gradient Descent : Example (Iteraion 14)



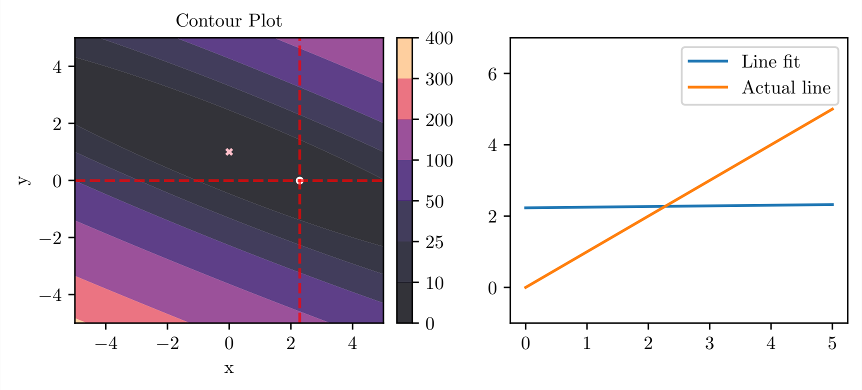
Gradient Descent : Example (Iteraion 16)



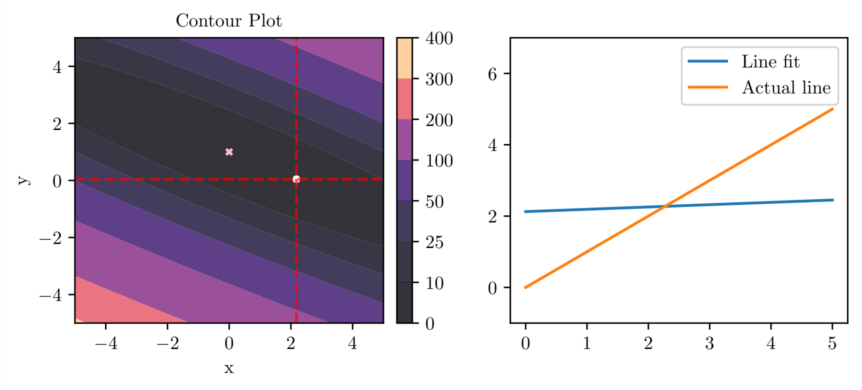
Gradient Descent : Example (Iteraion 18)



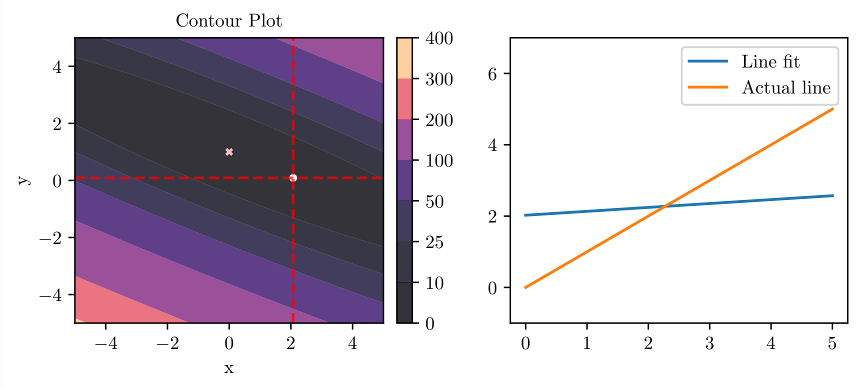
Gradient Descent : Example (Iteraion 20)



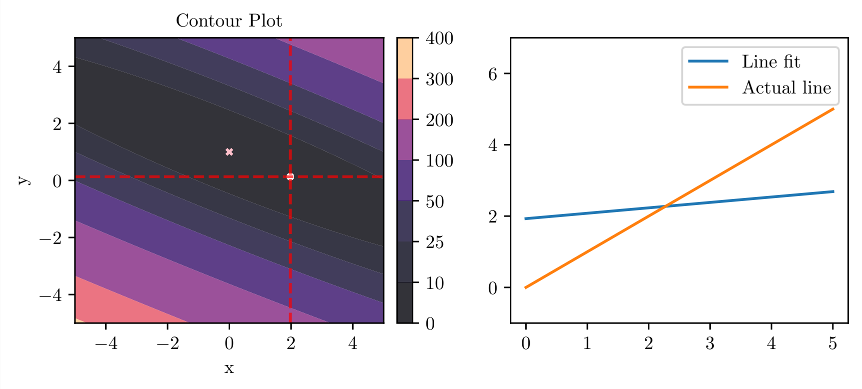
Gradient Descent : Example (Iteraion 22)



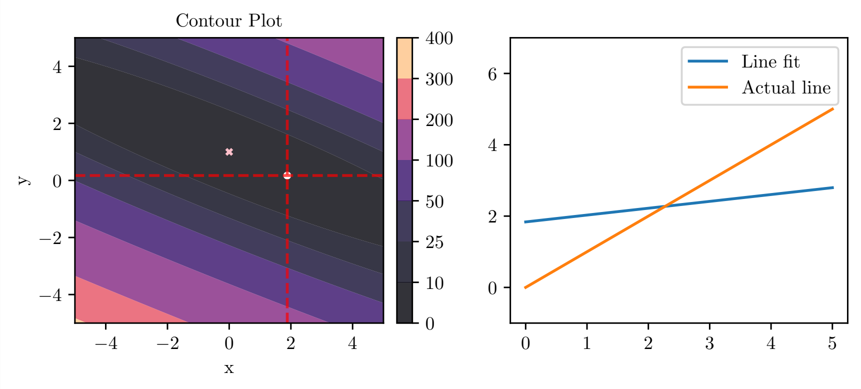
Gradient Descent : Example (Iteraion 24)



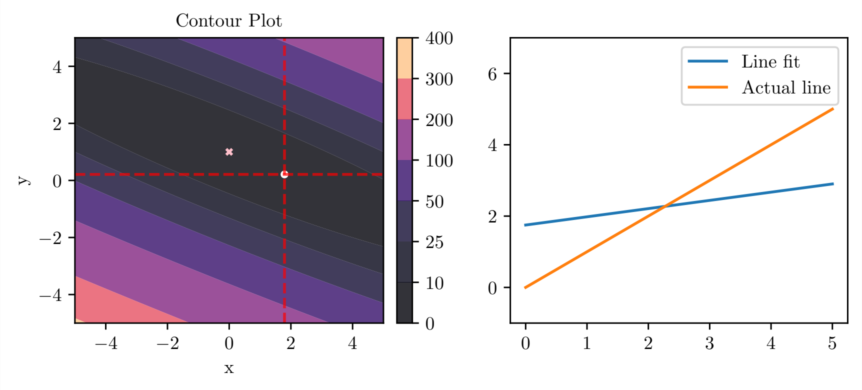
Gradient Descent : Example (Iteraion 26)



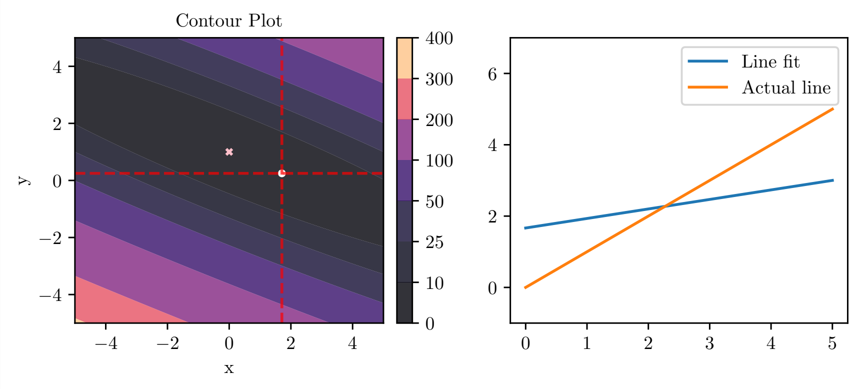
Gradient Descent : Example (Iteraion 28)



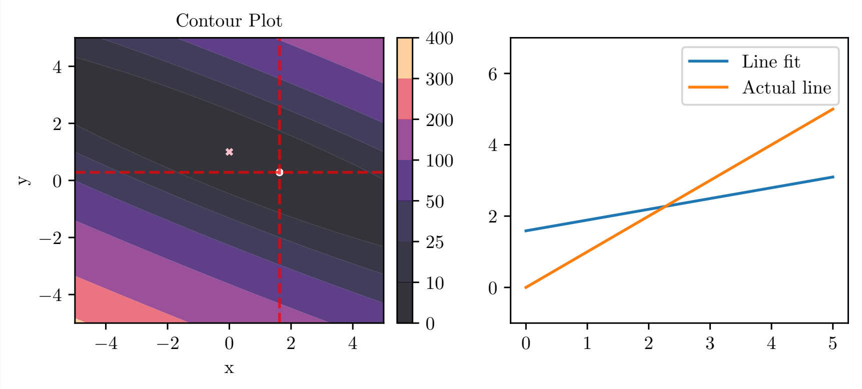
Gradient Descent : Example (Iteraion 30)



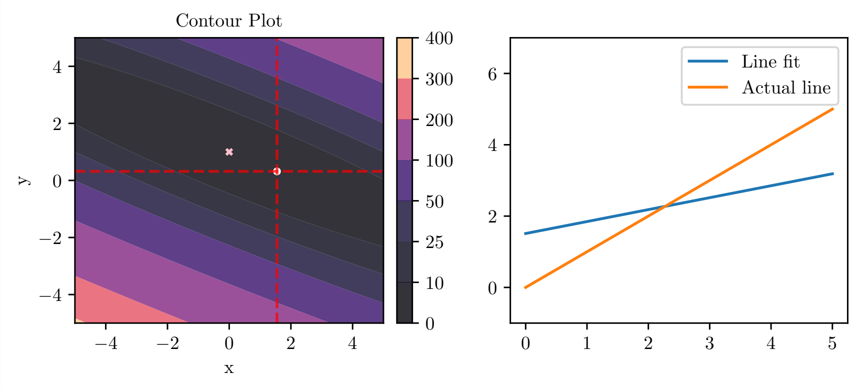
Gradient Descent : Example (Iteraion 32)



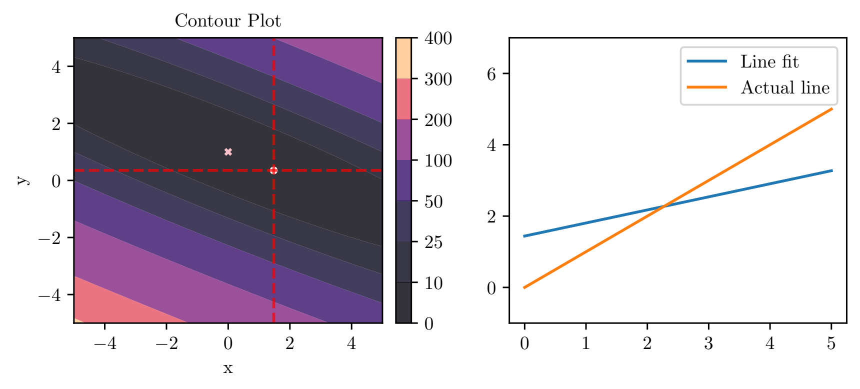
Gradient Descent : Example (Iteraion 34)



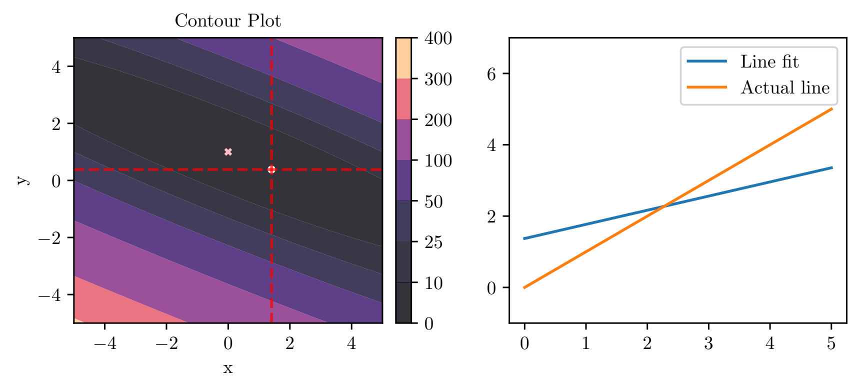
Gradient Descent : Example (Iteraion 36)



Gradient Descent : Example (Iteraion 38)



Gradient Descent : Example (Iteraion 40)



Iteration v/s Epcohs for gradient descent

- Iteration: Each time you update the parameters of the model

Iteration v/s Epcohs for gradient descent

- Iteration: Each time you update the parameters of the model
- Epoch: Each time you have seen all the set of examples

Gradient Descent (GD)

- Dataset: $D = \{(X, y)\}$ of size N
- Initialize θ
- For epoch e in $[1, E]$
  - Predict $\hat{y} = pred(X, \theta)$
  - Compute loss: $J(\theta) = loss(y, \hat{y})$
  - Compute gradient: $\nabla J(\theta) = grad(J)(\theta)$
  - Update: $\theta = \theta - \alpha \nabla J(\theta)$

Stochastic Gradient Descent (SGD)

- Dataset: $D = \{(X, y)\}$ of size N
- Initialize θ
- For epoch e in $[1, E]$
  - Shuffle D
  - For i in $[1, N]$
    - Predict $\hat{y}_i = pred(X_i, \theta)$
    - Compute loss: $J(\theta) = loss(y_i, \hat{y}_i)$
    - Compute gradient: $\nabla J(\theta) = grad(J)(\theta)$
    - Update: $\theta = \theta - \alpha \nabla J(\theta)$

Mini-Batch Gradient Descent (MBGD)

- Dataset: $D = \{(X, y)\}$ of size N
- Initialize θ
- For epoch e in $[1, E]$
  - Shuffle D
  - $Batches = make\_batches(D, B)$
  - For b in $Batches$
    - $X\_b, y\_b = b$
    - Predict $\hat{y\_b} = pred(X\_b, \theta)$
    - Compute loss: $J(\theta) = loss(y\_b, \hat{y\_b})$
    - Compute gradient: $\nabla J(\theta) = grad(J)(\theta)$
    - Update: $\theta = \theta - \alpha \nabla J(\theta)$

Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data

Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost

Gradient Descent vs SGD

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Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point

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- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point
- Noisier curve for iteration vs cost
- For a single update, it computes the gradient over one example. Hence lesser time

Stochastic Gradient Descent : Example

Learn $y = \theta_0 + \theta_1 x$ on following dataset, using SGD where initially $(\theta_0, \theta_1) = (4, 0)$ and step-size, $\alpha = 0.1$, for 1 epoch (3 iterations).

x	**y**
2	2
3	3
1	1

Stochastic Gradient Descent : Example

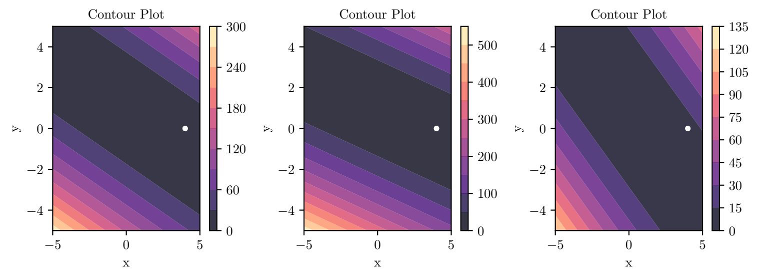
Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

Error for i^{th} datapoint, $e_i = y_i - \hat{y}_i$
$\epsilon_1 = 2 - \theta_0 - 2\theta_1$
$\epsilon_2 = 3 - \theta_0 - 3\theta_1$
$\epsilon_3 = 1 - \theta_0 - \theta_1$

While using SGD, we compute the MSE using only 1 datapoint per iteration.
So MSE is ϵ_1^2 for iteration 1 and ϵ_2^2 for iteration 2.

Stochastic Gradient Descent : Example

Contour plot of the cost functions for the three datapoints



Stochastic Gradient Descent : Example

For Iteration i

$$\frac{\partial MSE}{\partial \theta_0} = 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-1) = 2\epsilon_i\,(-1)$$

$$\frac{\partial MSE}{\partial \theta_1} = 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-x_i) = 2\epsilon_i\,(-x_i)$$

Stochastic Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.1 \times 2 \times (2 - (4 + 0))(-1)$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

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$$\theta_1 = 0 - 0.1 \times 2 \times (2 - (4 + 0))\,(-2)$$

$$\theta_1 = -0.8$$

Stochastic Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))(-1)$$

$$\theta_0 = 3.96$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))\,(-1)$$

$$\theta_0 = 3.96$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_0 = -0.8 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))\,(-3)$$

$$\theta_1 = 0.28$$

Stochastic Gradient Descent : Example

Iteration 3

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 3

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.96 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))(-1)$$

$$\theta_0 = 3.312$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 3

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.96 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))(-1)$$

$$\theta_0 = 3.312$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_0 = 0.28 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))(-1)$$

$$\theta_1 = -0.368$$

Stochastic gradient is an unbiased estimator of the true gradient

True Gradient

Based on Estimation Theory and Machine Learning by Florian Hartmann

- Let us say we have a dataset $\mathcal{D}$ containing input output pairs $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$

True Gradient

Based on Estimation Theory and Machine Learning by Florian Hartmann

- Let us say we have a dataset $\mathcal{D}$ containing input output pairs $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$
- We can define overall loss as:

$$L(\theta) = \frac{1}{N} \sum_{i=1}^{N} loss(f(x_i, \theta), y_i)$$

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- We can define overall loss as:

$$L(\theta) = \frac{1}{N}\sum_{i=1}^{N} loss(f(x_i, \theta), y_i)$$

- loss can be any loss function such as squared loss, cross-entropy loss etc.

$$loss(f(x_i, \theta), y_i) = (f(x_i, \theta) - y_i)^2$$

True Gradient

- The true gradient of the loss function is given by:

$$\begin{aligned}\nabla L &= \nabla \frac{1}{n}\sum_{i=1}^{n} \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\ &= \frac{1}{n}\sum_{i=1}^{n} \nabla \operatorname{loss}\left(f\left(x_i\right), y_i\right)\end{aligned}$$

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- The above is a consequence of linearity of the gradient operator.

Estimator for the true gradient

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- For SGD, we use a single example to estimate the true gradient, for mini-batch gradient descent, we use a mini-batch of examples to estimate the true gradient
- Let us say we have a sample: (x, y)
- The estimated gradient is given by:

$$\nabla \tilde{L} = \nabla \operatorname{loss}(f(x), y)$$

Bias of the estimator

- One measure for the quality of an estimator $\tilde{X}$ is its bias or how far off its estimate is on average from the true value X :

$$\text{bias}(X) = \mathbb{E}[\tilde{X}] - X$$

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- Using the rules of expectation, we can show that the expected value of the estimated gradient is the true gradient:

$$\begin{aligned}
\mathbb{E}[\nabla \tilde{L}] &= \sum_{i=1}^{n} \frac{1}{n} \nabla \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\
&= \frac{1}{n} \nabla \sum_{i=1}^{n} \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\
&= \nabla L
\end{aligned}$$

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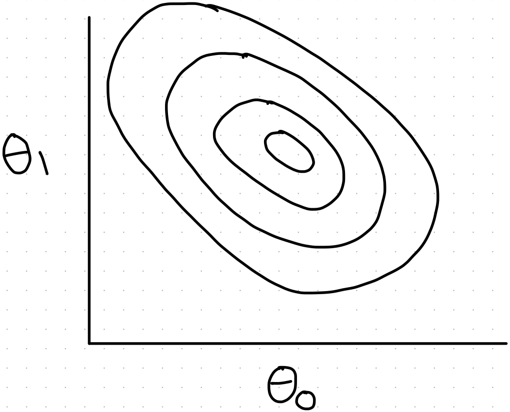
&= \frac{1}{n} \nabla \sum_{i=1}^{n} \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\
&= \nabla L
\end{aligned}$$

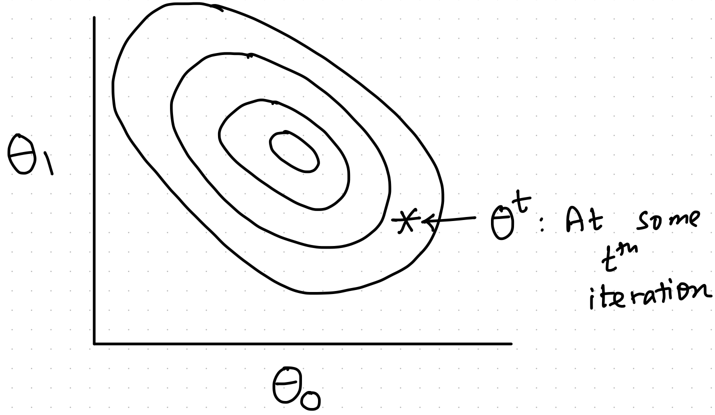
- Thus, the estimated gradient is an unbiased estimator of the true gradient

X	y
— x_1^T —	y_1
$\vdots$	
— x_N^T —	y_N

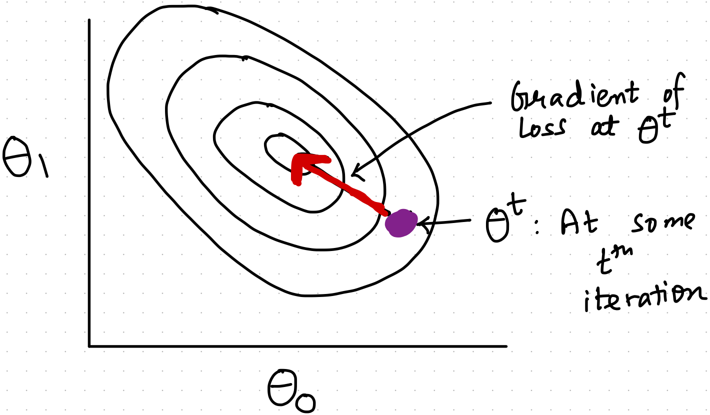
X	y	$\hat{y} = f(x, \theta)$
— x_1^T —	y_1	$\hat{y}_1$
$\vdots$		$\vdots$
— x_N^T —	y_N	$\hat{y}_N$



LOSS SURFACE OVER
6N' EXAMPLES



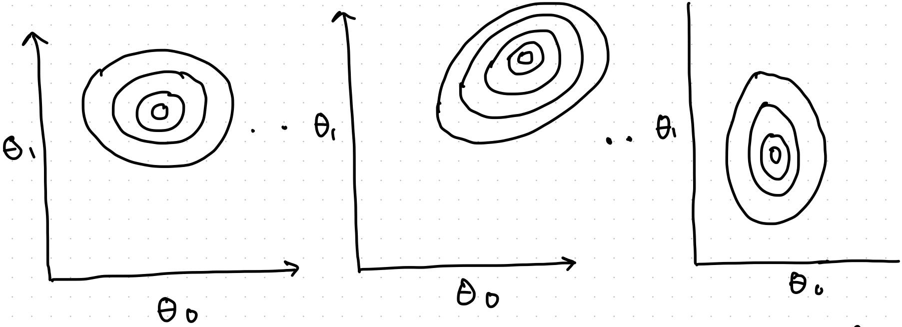
LOSS SURFACE OVER
6N' EXAMPLES



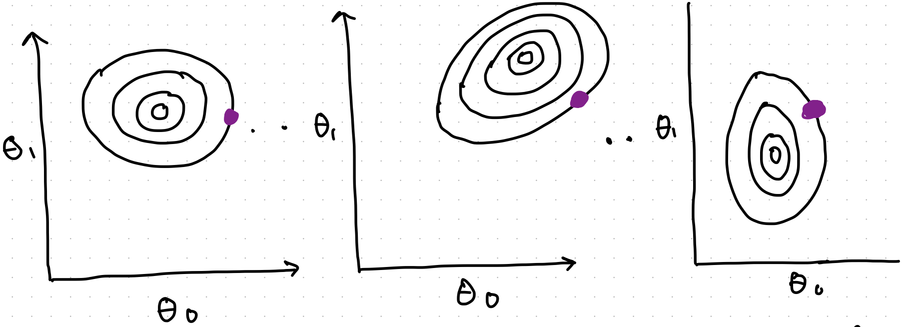
LOSS SURFACE OVER
6N° EXAMPLES

X	y	$\hat{y} = f(x, \theta)$
— x_1^T —	y_1	$\hat{y}_1$
$\vdots$		$\vdots$
$\vdots$		$\vdots$
— x_N^T —	y_N	$\hat{y}_N$

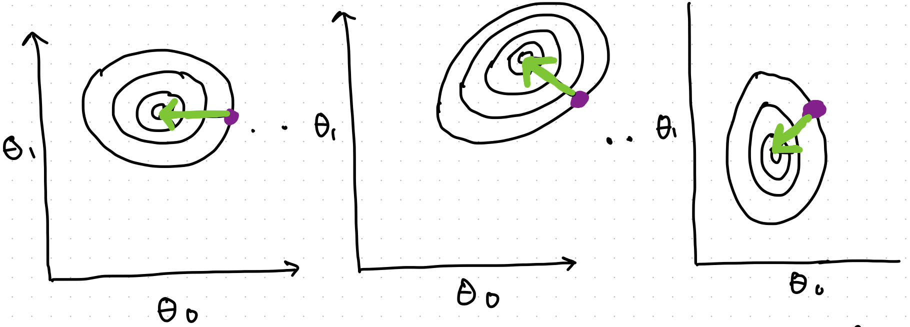
CONSIDER Individual data points to compute loss



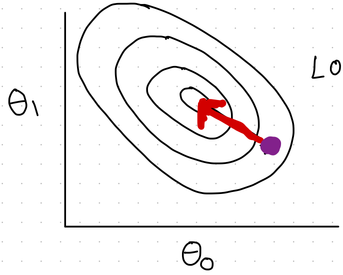
$loss(y_1, \hat{y}_1)$ $\qquad$ $loss(y_i, \hat{y}_i)$ $\qquad$ $loss(y_N, \hat{y}_N)$



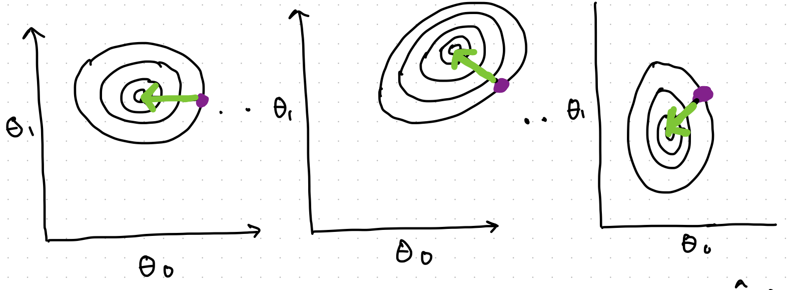
$loss(y_1, \hat{y}_1)$ $loss(y_i, \hat{y}_i)$ $loss(y_N, \hat{y}_N)$



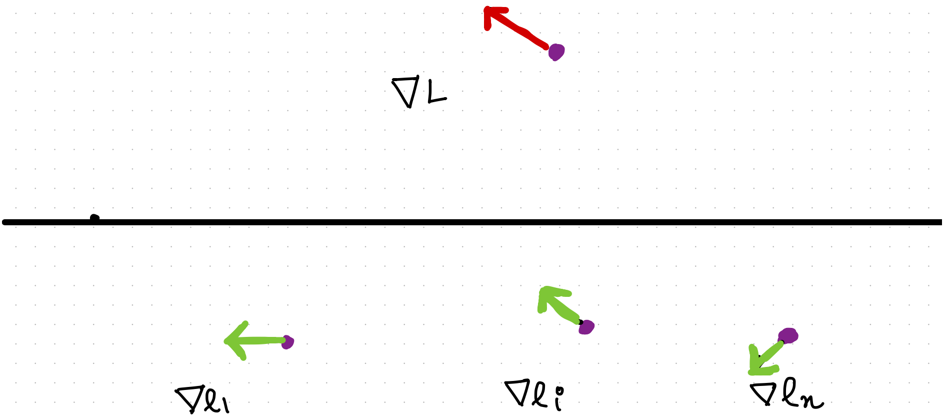
$loss(y_1, \hat{y}_1)$ $\quad$ $loss(y_i, \hat{y}_i)$ $\quad$ $loss(y_N, \hat{y}_N)$

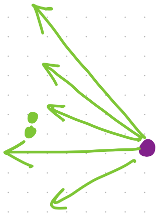


LOSS SURFACE OVER 'N' EXAMPLES

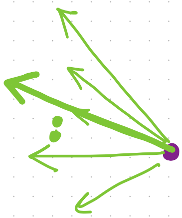


$loss(y_1, \hat{y}_1)$ $\quad$ $loss(y_i, \hat{y}_i)$ $\quad$ $loss(y_N, \hat{y}_N)$


∇L
∇l_1
∇l_i
∇l_n

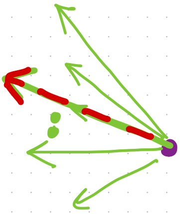


Gradients for losses wrt different points



Gradients for losses wrt different points

Expectation over individual gradients



Gradients for losses wrt different points

Expectation over individual gradients

Gradient wrt. whole data

Time Complexity: Gradient Descent v/s Normal Equation for Linear Regression

Normal Equation

- Consider $X \in \mathcal{R}^{N \times D}$

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- N examples and D dimensions

Normal Equation

- Consider $X \in \mathcal{R}^{N \times D}$
- N examples and D dimensions
- What is the time complexity of solving the normal equation $\hat{\theta} = (X^T X)^{-1} X^T y$?

Normal Equation

- X has dimensions $N \times D$, X^T has dimensions $D \times N$

Normal Equation

- X has dimensions $N \times D$, X^T has dimensions $D \times N$
- $X^T X$ is a matrix product of matrices of size: $D \times N$ and $N \times D$, which is $\mathcal{O}(D^2 N)$

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Normal Equation

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- $X^T y$ is a matrix vector product of size $D \times N$ and $N \times 1$, which is $\mathcal{O}(DN)$
- $(X^T X)^{-1} X^T y$ is a matrix product of a $D \times D$ matrix and $D \times 1$ matrix, which is $\mathcal{O}(D^2)$

Normal Equation

- X has dimensions $N \times D$, X^T has dimensions $D \times N$
- X^TX is a matrix product of matrices of size: $D \times N$ and $N \times D$, which is $\mathcal{O}(D^2N)$
- Inversion of X^TX is an inversion of a $D \times D$ matrix, which is $\mathcal{O}(D^3)$
- X^Ty is a matrix vector product of size $D \times N$ and $N \times 1$, which is $\mathcal{O}(DN)$
- $(X^TX)^{-1}X^Ty$ is a matrix product of a $D \times D$ matrix and $D \times 1$ matrix, which is $\mathcal{O}(D^2)$
- Overall complexity: $\mathcal{O}(D^2N) + \mathcal{O}(D^3) + \mathcal{O}(DN) + \mathcal{O}(D^2)$ $= \mathcal{O}(D^2N) + \mathcal{O}(D^3)$

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- Scales cubic in the number of columns/features of X

Gradient Descent

Start with random values of θ_0 and θ_1

Till convergence

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- $\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} (y - X\theta)^\top (y - X\theta)$
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  $\theta_D = \theta_D - \alpha \frac{\partial}{\partial \theta_D} (y - X\theta)^\top (y - X\theta)$

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- $\theta = \theta - \alpha \frac{\partial}{\partial \theta} (y - X\theta)^\top (y - X\theta)$

Gradient Descent

$$
\begin{aligned}
&\tfrac{\partial}{\partial\theta}(y - X\theta)^\top (y - X\theta) \\
&= \tfrac{\partial}{\partial\theta}\left(y^\top - \theta^\top X^\top\right)(y - X\theta) \\
&= \tfrac{\partial}{\partial\theta}\left(y^\top y - \theta^\top X^\top y - y^\top x\theta + \theta^\top X^\top X\theta\right) \\
&= -2X^\top y + 2X^\top x\theta \\
&= 2X^\top (X\theta - y)
\end{aligned}
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All of the above need only be calculated once!

Gradient Descent

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For each of the t iterations, we now need to first multiply $\alpha X^\top X$ with θ which is matrix multiplication of a $D \times D$ matrix with a $D \times 1$, which is $\mathcal{O}(D^2)$

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$\mathcal{O}(tD^2) + \mathcal{O}(D^2N) = \mathcal{O}((t+N)D^2)$

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- Computing $\theta = \theta - \alpha X^{\top}(X\theta - y)$ is $\mathcal{O}(N)$

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$\mathcal{O}(NDt)$